

Formaldehyde-(14)C
3046-49-9 | DTXSID20184538

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.93 | 22.5 | 0.93 | 22.1 | 0.93 | 22.1 |

Model Results

Predicted value: -6.27 °C

Global applicability domain: Inside

Local applicability domain index: 5.75e-01

Confidence level: 8.85e-01

Nearest Neighbors from the Training Set

| | | |
|---|---|---|
| <div>Image not found</div> <div>Formaldehyde</div> <div>Measured: -19.1</div> <div>Predicted: -19.9</div> | <div>Image not found</div> <div>Dimethyl ether</div> <div>Measured: -24.8</div> <div>Predicted: -26.1</div> | <div>Image not found</div> <div>Acetaldehyde</div> <div>Measured: 20.1</div> <div>Predicted: 23.9</div> |
| <div>Image not found</div> <div>Ethylene oxide</div> <div>Measured: 10.6</div> <div>Predicted: 11.9</div> | <div>Image not found</div> <div>Chloroethane</div> <div>Measured: 12.3</div> <div>Predicted: 8.50</div> | |